Computation of Poisson-Nernst-Planck Equations Describing Ion Channel on Cell Membrane

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Introduction

Ion channels are proteins with a hole down the middle embedded in cell membranes allowing and controlling the movement of charged particles, mostly Na+, K+, Ca++, and Cl-. The traditional continuum model for ion channel is Poisson-Nernst-Planck (PNP) equations. Though PNP equations can produce some results and agree well with experiments, this model still can not explain channel gating and selectivity. This may be because finite-size effect is not included in traditional PNP model to address the crowdedness in channel filter.

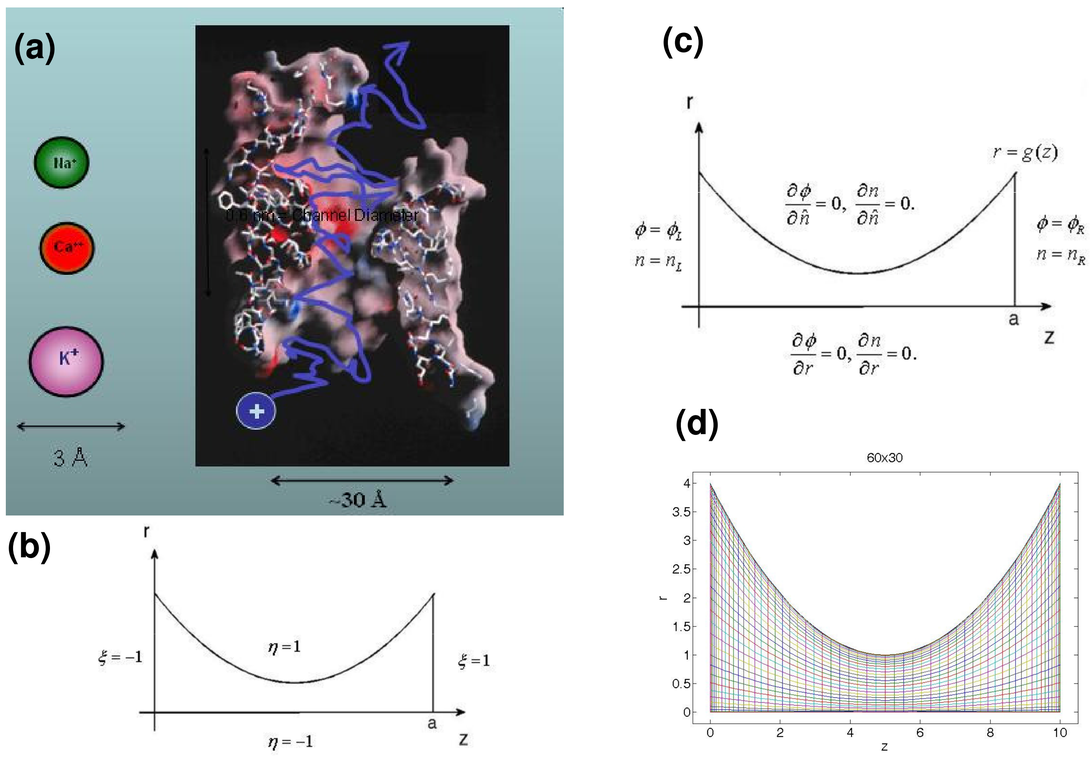

Figure 1. (a) A typical ion channel structure. (b) Axis-symmetric reduced model. (c) Boundary conditions. (d) Chebysehv-Gauss-Lobatto mesh.

Mathematical model

The governing equations are modified PNP equations with finite-size effect characterized by Leonard-Jones potential [1].

$$E^{total}=\int\left(k_BT\sum_{i=1}^{N}c_i\log c_i+(\rho_0+z_iec_i)\phi+M_{O^{-1/2}}(\psi+1)c_{O^{-1/2}}\right)d\vec{x}$$
$$+\int c_i(\vec{x})\sum_{j=1}^{N}\int\frac{\varepsilon_{i,j}}{2}\frac{(a_i+a_j)^{12}}{|\vec{x}-\vec{y}|^{12}}c_j(\vec{y})d\vec{y}\,d\vec{x} \qquad (1.1)$$

$$\frac{\partial c_i}{\partial t}=\nabla\cdot\left[D_i\left\{\nabla c_i+\frac{c_i}{k_BT}\left(z_ie\nabla\phi+\sum_{j=1}^{N}\nabla\int\frac{c_0\varepsilon_{i,j}(a_i+a_j)^{12}}{|\vec{x}-\vec{y}|^{12}}c_j(\vec{y})\,d\vec{y}\right)+M_ic_i\nabla\psi\right\}\right]$$
$$-\nabla\cdot(\varepsilon\nabla\phi)=\rho_0+\sum_{i=1}^{N}z_iec_i,\quad \text{for } i,j=1,\cdots,N, \qquad (1.2)$$

Numerical method

Eqs. (1.1-1.2) are computed under the framework of method of lines (MOL). The actual ion channel like Fig. 1(a) is here simplified to a funnel as shown in Fig. 1(b) [2]. This axis-symmetric geometric configuration is further mapped to a rectangular domain. Eqs. (1.1-1.2) after coordinate transformation are spatially discretized by the highly accurate Gauss-Lobatto Chebyshev pseudospectral method, and integrated in time by MATLAB script ode15s with the boundary conditions shown in Fig. 1(c). The mesh in physical domain is shown in Fig. 1(d). The Poisson equation in (1.2) can be solved by a Poisson solver. If only steady state solution of Eqs. (1.1-1.2) are cared, an artificial time derivative term can be added to the Poisson equation and make it parabolically time-dependent, which is more efficient to compute.

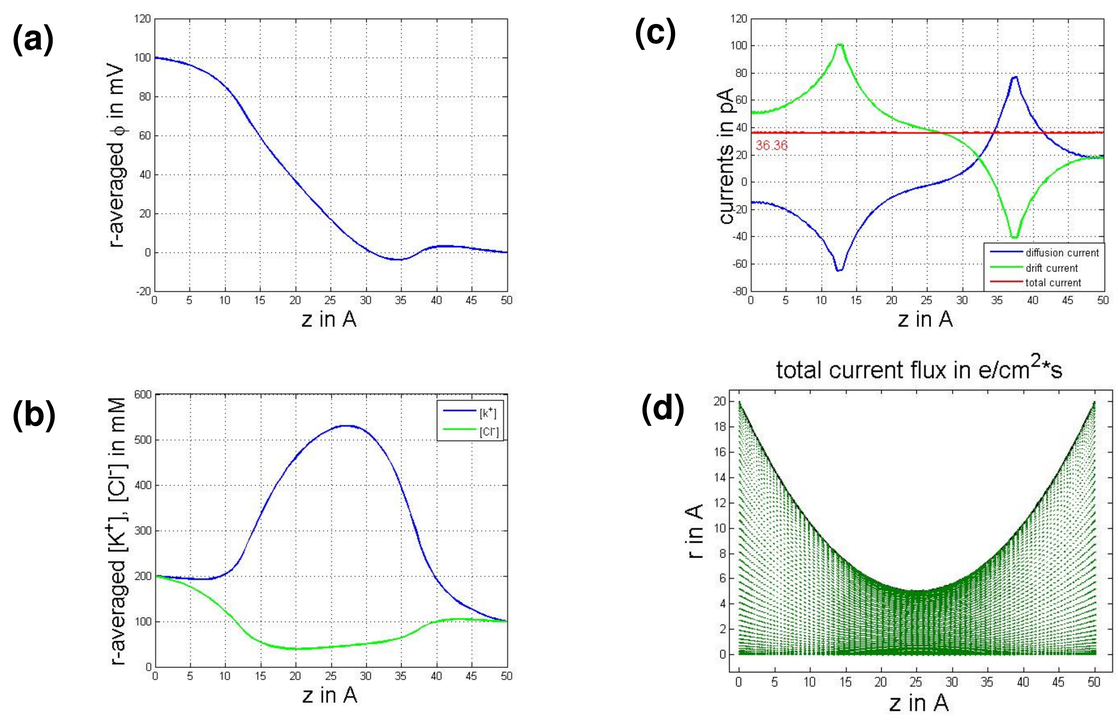

Figure 3. 1D distribution of (a) electric potential, (b) potassium and chloride ion concentration, under cross-sectional average. (c) Diffusion, drift and total currents. (d) Current flux vector diagram.

Results and discussions

One permanent charge -1e from side-chain of channel protein is placed in the narrowest part of channel (filter). The computation results are shown in Figs. (2) and (3). In Fig. 2(c), ion fluxes are integrated for the whole cross-section area at each z location to obtain diffusion, drift, and total currents, respectively.

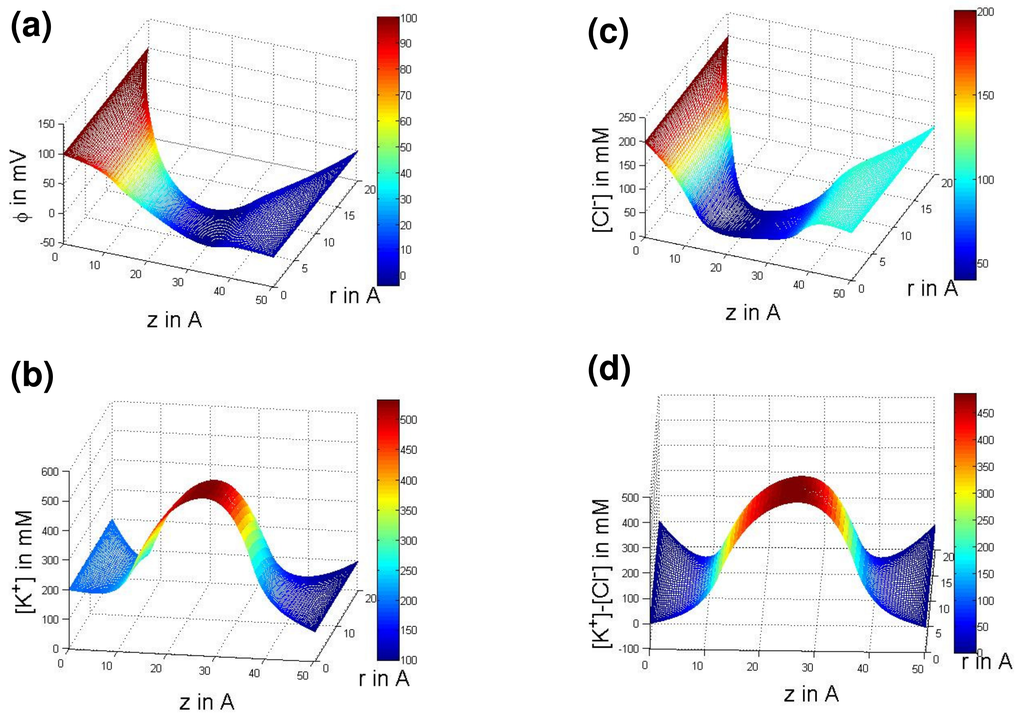

Figure 2. Distribution of (a) electric potential, (b) potassium ion concentration, (c) Chloride ion concentration, (d) The difference between potassium and chloride ion concentrations.

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[2] A. Singer and J. Norbury, A Poisson–Nernst–Planck model for biological ion channels-an asymptotic analysis in a three-dimensional narrow funnel, SIAM J. Appl. Math., 70(3):949-968, 2009.